Proposed term project for PHY 381C: Computational Physics

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Numerical solution of the time-dependent Schrödinger equation for a 2D electron waveguide

The behavior of electrons in a 2D waveguide with a cavity like the one shown in Fig. 1 is described by the two-dimensional Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\Psi + V\Psi \tag{1}$$

with the boundary conditions that Ψ vanishes at $x_2 = \pm(w + h\xi(x_1))$, open

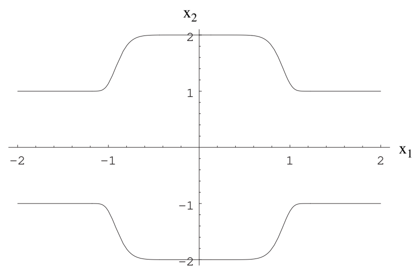

Figure 1: 2D waveguide with a cavity

boundaries in x_1-direction and Ψ, V both dependent on time and two spatial coordinates. If the boundary is chosen to be analytic, one can transform (1) using the coordinate transformation $x_1 = u_1, x_2 = (w + h\xi(u_1))\, v$ to

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}g^{-1/2}\frac{\partial}{\partial u_i}\left(g^{1/2}g^{ij}\frac{\partial\Psi}{\partial u_j}\right)\Psi + V\Psi \tag{2}$$

with the metric tensor

$$g_{ij} = (w + h\xi(u_1))\begin{pmatrix} \frac{1+h^2u_2^2\dot{\xi}^2(u_1)}{w+h\xi(u_1)} & hu_2\dot{\xi}(u_1) \\ hu_2\xi(u_1) & w + h\xi(u_1) \end{pmatrix} \tag{3}$$

and the simpler boundary conditions that Ψ vanishes at $u_2 = \pm 1$. ξ can be chosen to model the cavity, e.g. $\xi(x) = e^{-\frac{x^{2p}}{2\sigma^2}}$ with appropriate values of p and σ.

The goal of my term project is to implement a finite difference algorithm to solve eq. (2) numerically and look at the transmission properties of the waveguide (with and without an external potential).